

High Temperature Single Crystal X-ray Structure of $\text{Ca}_2\text{Fe}_2\text{O}_5$

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Beamline(s): X7B

Introduction: The ferrite solid solution series $\text{Ca}_2(\text{Fe}_{1-x}\text{Al}_x)_2\text{O}_5$ is one of the four major phases in Portland cement clinkers. Differential thermal analysis (DTA) in this system revealed two very weak signals at about $T_1=443^\circ\text{C}$ and $T_2=688^\circ\text{C}$. The present investigation was focussed on the end member $\text{Ca}_2\text{Fe}_2\text{O}_5$ and was aimed to characterize these transitions in more detail.

Methods and Materials: The data was collected with a mar345 image plate detector at 25°C and 500°C . The sample was rotated in a u-shaped resistive heater. Data were reduced with the HKL programs¹ with an additional correction to account for incomplete adsorption in the phosphor layer of the image plate². The structures were refined with SHELXL-93³ (25°C $R_1=0.018$, $wR_2=0.056$ 188refl.), (500°C $R_1=0.022$, $wR_2=0.066$ 194 reflections.)

Results: The comparison of the structure refinements below and above the first transition indicates that the two structures are isotypic. No change in space group symmetry could be observed. The first transition is a pure magnetic one and the signal in the DTA at 443°C corresponds to the loss of the anti-ferromagnetic ordering of the magnetic moments of the Fe^{3+} cations.

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References: 1. Z. Otwinowski and W. Minor, *Methods in Enzymology*, Vol. **276**: Macromolecular Crystallography, Part A, 307-326, (1997) C.W. Carter, Jr. & R.M. Sweet, Eds. Academic Press; 2. J. Zaleski *et al.* *J. Appl. Cryst.* **31**, 302-304; 3. G.M. Sheldrick, SHELXL-93 University of Göttingen, Germany, 1993.

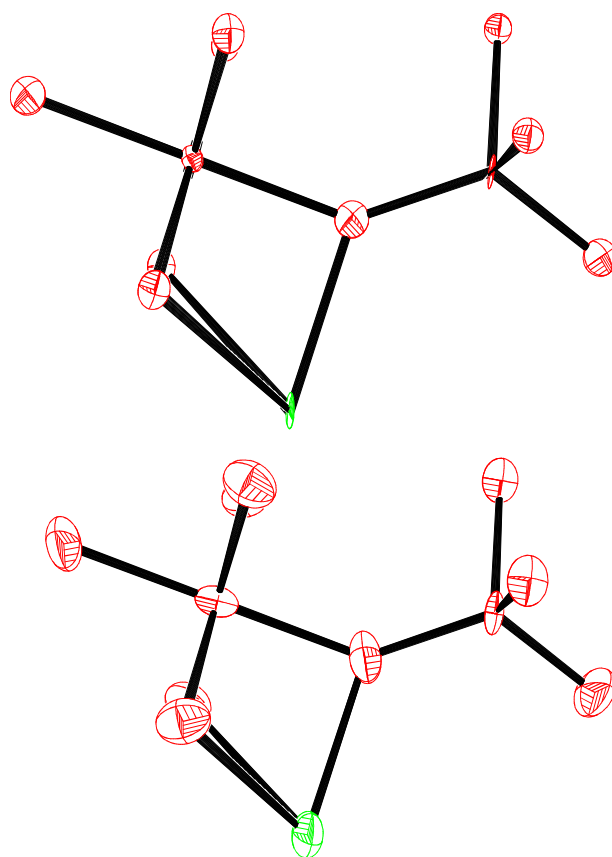


Figure 1. Thermal ellipsoid plot of part of the structure. Top figure is at 25°C and bottom figure is at 500°C . The thermal motion ellipsoids are plotted at the 90% probability level because they are so small. The thermal motion increases with temperature as expected.